A linearized spin-wave theory for thermodynamics of quantum Heisenberg antiferromagnet on a square lattice

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(Dated: December 25, 2009)

The thermodynamics of the quantum Heisenberg antiferromagnet on a square lattice is revisited through a linearized spin-wave theory which is well defined at any finite temperature. We re-examine in details the temperature dependence of the free energy, the internal energy, the entropy and the specific heat. Most conclusions of the thermodynamics in previous studies can be reproduced in our linearized spin-wave theory. Specially, our calculation at low temperature $T < J$ agrees quantitatively with the numerical Quantum Monte Carlo simulation and high temperature series expansions.

PACS numbers: 75.30.Ds, 75.40.Cx, 75.50.Ee

The two-dimensional (2D) quantum magnets is one of the main subjects in the modern condensed matter physics, as they are closely related to the unconventional superconductivity in the cuprates[1] and the novel quantum spin-liquid states in frustrated lattices.[2] The previous studies are mainly concentrated in the low-energy physics. However, some interesting physics, such as the crossover behavior[3] in 2D quantum Heisenberg antiferromagnet (QHAFM) and the pseudogap physics in the cuprates,[4] occurs at high energy scales and are still in controversial. One reason for these controversies is the lack of a reliable theoretical formalism well-defined in full temperature region.

Recently we proposed a perturbation spin-wave theory for the 2D QHAFM on a square lattice.[5] Our theory is based upon Takahashi's modified spin-wave theory, where in order to study the finite temperature disordered state, he introduced a constraint of the loss of the local moment.[6] It is found that the 2D quantum antiferromagnet is well described at low temperatures by this modified spin-wave theory, yielding the results consistent to the other theories[7, 8, 9] and numerical simulations.[6, 10, 11] In the modified spin-wave theory, a mean-field ansatz is introduced to decouple the spin-wave interactions. Although it gives a good description of the low-energy physics, it results in the failure of the theory at high temperatures $T \simeq J$, where an artificial phase transition occurs which obviously violates the Mermin-Wagner theorem.[12]

In our perturbation spin-wave theory, the loss of the local moment is also included to fulfill the Mermin-Wagner theorem. The corrections from the spin-wave interactions are studied via a many-body perturbation method, which removes the mean-field divergence in the modified spin-wave theory. The temperature dependence of the uniform static susceptibility from our perturbation spin-wave theory agrees well with the quantum Monte Carlo simulations and high temperature series expansions.[5] It shows that our theory is well-defined at any finite temperature and is a good formalism for the 2D QHAFM. Moreover it is found that even the linearized spin-wave theory with the spin-wave interactions neglected can reproduce the main features of the uniform static susceptibility. Thus it encourages us to use the linearized spin-wave theory, on its reliability and simplicity, to study the thermodynamical properties of 2D QHAFM.

In this paper, we present our calculations of the thermodynamical variables of a QHAFM on a square lattice, including the free energy, the internal energy, the entropy and the specific heat. Comparing with the numerical simulations, it shows that the linearized spin-wave theory can also reproduce nearly all of the features in thermodynamics. At low temperature $T < J$, our calculations of the internal energy and the specific heat agree quantitatively with the quantum Monte Carlo simulations and high temperature series expansions.

The Hamiltonian of a QHAFM on a square lattice is given by

$$H_s = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{1}$$

where $J > 0$ and $\langle ij \rangle$ denotes nearest-neighbor sites. Since the ground state is a Néel ordered state, we separate the lattice (with $2N$ sites) into two sublattice, where sublattice A (B) is defined for the up (down) spins in the Néel order state.
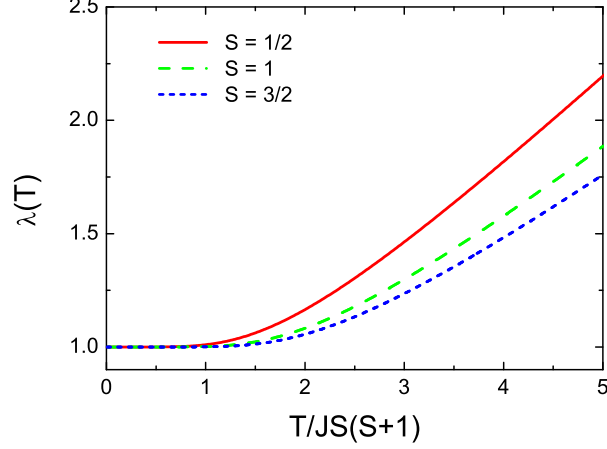
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FIG. 1: The temperature dependence of the Lagrange multiplier λ in our linearized spin-wave theory of QHAFM on a square lattice with spins $S = 1/2, 1$ and $3/2$.

Following Takahashi, we introduce a Lagrange constraint into the Hamiltonian,[6]

$$H_\lambda = - \sum_{l \in A, B} \mu_l S_l^z. \tag{2}$$

The lagrange multipliers are assumed as $\mu_l = \mu$ if $l \in A$ and $-\mu$ if $l \in B$, and μ is re-defined as $\mu \equiv JzS(\lambda - 1)$ for convenience in our following discussion. This Lagrange Hamiltonian fulfills the Mermin-Wagner theorem for the loss of the local magnetization. It leads to a finite gap in the spin-wave energy spectrum and thus the spin-wave excitations behave as bosons with finite mass at finite temperatures.

In our spin-wave theory, the spin operators are expressed by bosonic operators based upon the Dyson-Maleev representation,[6]

$$S_i^- = a_i^\dagger, S_i^+ = (2S - a_i^\dagger a_i)a_i, S_i^z = S - a_i^\dagger a_i, \tag{3}$$

for the spins in sublattice A and

$$S_j^- = b_j, S_j^+ = b_j^\dagger(2S - b_j^\dagger b_j), S_j^z = -S + b_j^\dagger b_j, \tag{4}$$

in sublattice B. With this spin representation, the Hamiltonian $H = H_s + H_\lambda$ can be expressed as summation of quadratic and quantic terms in these bosonic operators. In our following discussion, we will neglect the quantic terms which represent the spin-wave interactions and investigate the thermodynamics of QHAFM within a linearized spin-wave theory. The quadratic linearized spin-wave terms in the Hamiltonian can be easily diagonalized through the Fourier and Bogoliubov transformations. The free energy per site is readily obtained as[5]

$$\begin{aligned} F &= \frac{T}{N} \sum_{\mathbf{k}} \ln \left(2 \sinh \left(\frac{\varepsilon_{\mathbf{k}}}{2T} \right) \right) - \frac{1}{2} Jz\lambda S(1 + 2S) \\ &\quad + \frac{1}{2} JzS^2, \end{aligned} \tag{5}$$

where the spin-wave spectrum $\varepsilon_{\mathbf{k}} = JzS\sqrt{\lambda^2 - \gamma_{\mathbf{k}}^2}$ and $\gamma_{\mathbf{k}} = \cos \frac{1}{2}k_x \cos \frac{1}{2}k_y$. $z = 4$ is the coordinate number.

The parameter λ is unknown and determined by the free energy. Minimizing the free energy with respect to λ leads to a self-consistent equation for it,[5]

$$S = -\frac{1}{2} + \frac{1}{2N} \sum_{\mathbf{k}} \coth \left(\frac{\varepsilon_{\mathbf{k}}}{2T} \right) \frac{\lambda}{\sqrt{\lambda^2 - \gamma_{\mathbf{k}}^2}}. \tag{6}$$

The numerical calculation of the self-consistent equation Eq.(6) has been present in details in our previous paper.[5] Here we only cite the main results. The temperature dependence of the Lagrange multiplier λ is shown in Fig.
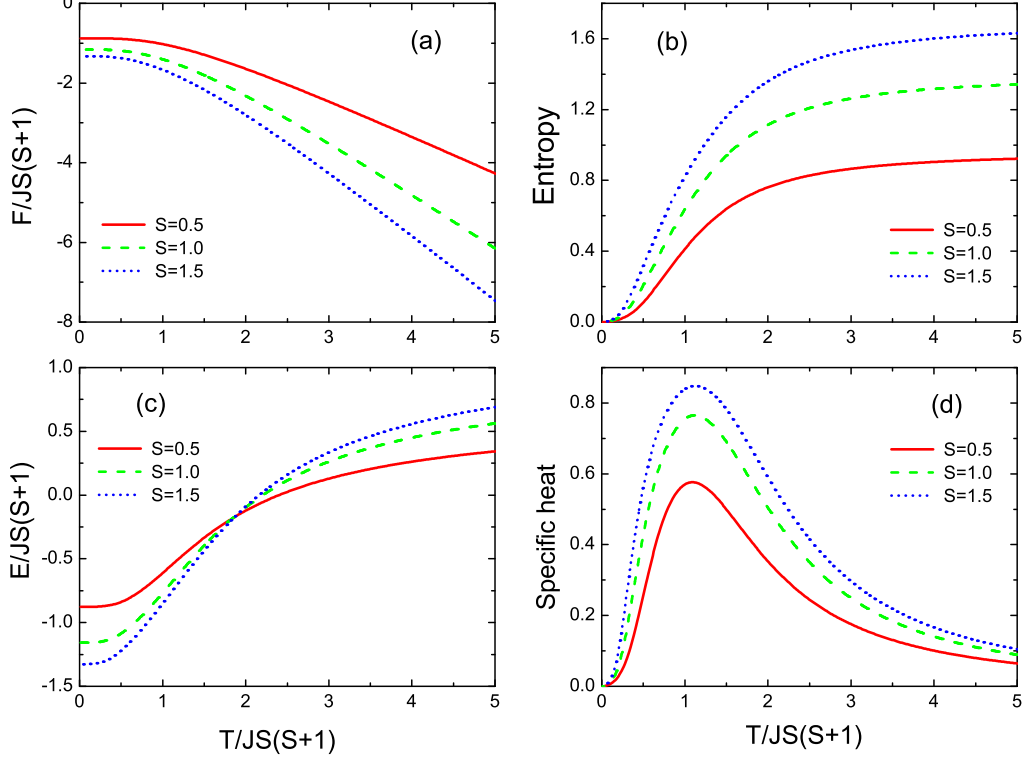
FIG. 2: Thermodynamics of the QHAFM on a square lattice with different spin magnitudes, $S = 1/2, 1$ and $3/2$. (a) is the free energy per site, (b) the entropy, (c) the internal energy and (d) the specific heat.

1. At zero temperature the spin waves condensate to the momentum $(0,0)$ which results in a long-range magnetic order.[6, 13] In this case, $\lambda = 1 + O(1/N)$ and the spin-wave excitation is gapless. At low but finite temperatures, the long-range order is destroyed by the quantum fluctuations.[12] Then λ has an exponential behavior and decays to its zero-temperature value 1 as $\lambda = 1 + \frac{1}{2}\left(\frac{T}{JzS}\right)^2 \exp\left(-\frac{\pi JzSm_0}{T}\right)$. Here $m_0 = S - 0.19660$ is the spontaneous ordered moment at zero temperature. The spin waves thus behaves as bosons with a finite gap $\Delta = \sqrt{\lambda^2 - 1}$. It is this finite gap that leads to the vanishing of the long-range magnetic order at any finite temperature. At high temperatures, the self-consistent equation gives a weak dispersion for the spin waves with $\lambda = \frac{T}{JzS}\ln\left(1 + \frac{1}{S}\right)$.

After the temperature variation of λ is obtained, we have calculated the uniform static magnetic susceptibility in our previous paper.[5] Now let us turn our attention into the thermodynamical properties. Fig. 2 shows the temperature dependence of the free energy, the entropy, the internal energy and the specific heat of the QHAFM on a square lattice. The free energy per site is obtained from Eq.(5). In low temperature region,

$$F(T) = -\frac{1}{2}JzS(S + 0.157948) + cT^3.$$

where c is a S-dependence constant. At high temperatures, it decreases linearly with temperature,

$$F = -T\ln\left[(1+S)\left(1+S^{-1}\right)^S\right] + \frac{1}{2}JzS^2.$$

This high-temperature behavior has been obtained by Takahashi,[6] where the last constant term does not exist. Based on the good agreement of our internal energy and specific heat with the numerical simulations as discussed below, we argue that the finite constant term in our theory comes from the linearized approximation.

The entropy shown in Fig. 2 (b) is is calculated from

$$\mathcal{S}_n = \frac{1}{N} \sum_{\mathbf{k}} \left[(n_{\mathbf{k}} + 1) \ln (n_{\mathbf{k}} + 1) - n_{\mathbf{k}} \ln n_{\mathbf{k}} \right], \tag{7}$$

where $n_{\mathbf{k}} = \frac{1}{e^{\varepsilon_{\mathbf{k}}/T} - 1}$. At zero temperature, the entropy is zero, which is consistent to the second law of the thermodynamics. It shows a square law $\sim T^2$ as temperature increases. When temperature is high enough, it approaches a constant value

$$\mathcal{S}_n = \ln \left[(1 + S) \left(1 + S^{-1} \right)^S \right].$$

This value is different from $\ln (2S + 1)$. It is also due to the neglect of the spin-wave interactions in our theory.

The internal energy is calculated from the free energy and entropy as $E = F + T\mathcal{S}_n$. At zero temperature for spin-1/2, our calculation gives $E = -0.657948$. It is quite close to the value -0.669494 which has included the spin-wave interaction corrections,[14] and -0.669437 in quantum Monte Carlo simulation.[15] It shows that the spin-wave interactions have a very weak contribution to the internal energy at low temperatures. When temperature increases, the free energy increases with an approximate T^3-law and finally approaches a constant value at high enough temperature. This asymptotic behavior has also be shown in the high temperature series expansions.[16] A slight difference is that there is constant value $E = \frac{1}{2} JzS^2$ in our theory, but it is zero in high temperature series method. This difference stems from our linearized approximation. A detailed comparison of the internal energy from our linearized spin-wave theory with the quantum Monte Carlo simulation and high-temperature series study is shown in Fig. 3 (a). A good agreement at temperature $T < JS(S + 1)$ shows that the spin-wave interactions has ignorable contribution to the internal energy at low temperatures.

The specific heat can be calculated from $C_v = T \frac{\partial \mathcal{S}_n}{\partial T}$ which leads to the following expression,

$$C_v = \frac{1}{4NT^2} \sum_{\mathbf{k}} \frac{\varepsilon_{\mathbf{k}}^2 - (JzS)^2 \lambda T \frac{\partial \lambda}{\partial T}}{\sinh^2 (\varepsilon_{\mathbf{k}}/2T)}. \tag{8}$$

Here $\frac{\partial \lambda}{\partial T}$ can be obtained by the derivative of both sides of the self-consistent equation Eq.(6). The temperature dependence of the specific heat is shown in Fig. 2 (d). It vanishes at zero temperature and shows an approximate T^2-law at low temperatures. It exhibits a broad peak at intermediate temperature $T \simeq JS(S + 1)$ and then decreases as bT^{-2} at high temperature. A more detailed analyses of our numerical data shows that $b = 0.9075$ for $S = \frac{1}{2}$. Both the low temperature T^2 behavior and T^{-2} decay at high temperatures are consistent to the high temperature series expansions.[17] The comparison with the numerical simulations is given in Fig. 3 (b). It shows that our linearized spin-wave theory has grasped main features in the specific heat: a low temperature T^2 behavior, a smooth crossover broad peak at intermediate temperature and a high temperature T^{-2} decrease. A detailed comparison shows that at low temperature $T < JS(S + 1)$, our linearized spin-wave theory agree quantitatively with the numerical simulations, which indicates the validity of the spin-wave formalism in studying the thermodynamics of the QHAFM.

I. SUMMARY

In summary, we have calculated the thermodynamical quantities of the QHAFM model on a square lattice from our linearized spin-wave theory. Our calculations include the free energy, the entropy, the internal energy and the specific heat. Although the neglect of the spin-wave interactions in our theory leads to some difference in magnitude compared to the numerical simulations, it has captured main features of the thermodynamics. The quantitative agreement of the internal energy and specific heat with the numerical simulations at low temperature $T < JS(S + 1)$ indicates that the spin-wave theory is an appropriate formalism to study the 2D QHAFM model.

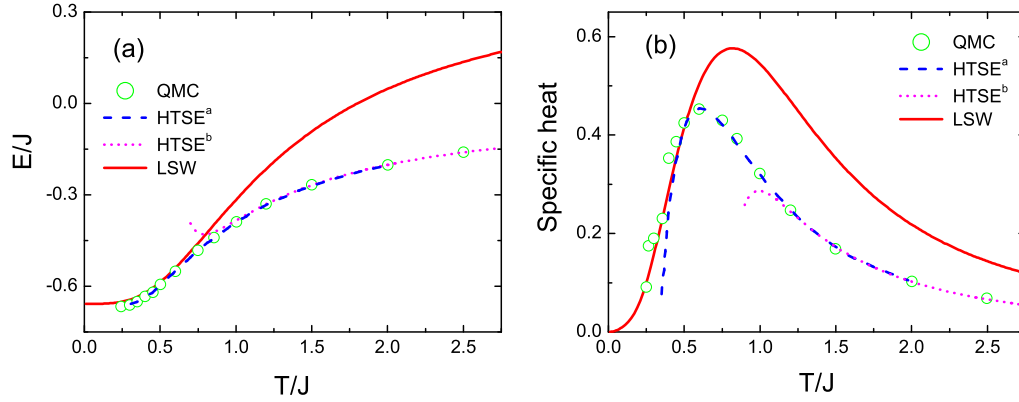[1] E. Manousakis, Rev. Mod. Phys. **63**, 1 (1991).

FIG. 3: Comparisons of the internal energy and the specific heat from our linearized spin-wave theory (LSW) to the quantum Monte Carlo (QMC) and high temperature series expansions (HTSE). Here QMC data comes from Ref. [10] and HTSE^a from a method with Padé approximation in Ref. [16] and HTSE^b from the formula Eq.(1) in the same reference.

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